FHKL– a program to compute rocking curves and crystallographic data of interest for the dynamical theory of X-rays

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FHKL – a program to compute rocking curves and crystallographic data of interest for the dynamical theory of X-rays.

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The crystallographic problem: Crystallographers working in fields such as topography or monochromator design with a conventional X-ray source or, more often nowadays, with a synchrotron beam need to compute crystal characteristics: dielectric susceptibilities χ (*via* structure factors), absorption coefficients μ/ρ and crystal rocking curves. These computations must be performed to a good precision, taking into account dispersion correction (f' and f''), polarization and the dynamical theory for rocking curves.

People generally use a set of rather inconvenient heterogeneous programs for these computations which are not always very user-friendly.

Method of solution: *FHKL* is a very easy to use menu-driven program: the user enters data and chooses options by clicking on buttons or moving sliders with a mouse inside the X-window graphical interface. The program needs only one data file containing information about the atoms of the asymmetric unit of the crystal.

FHKL may perform the following tasks:

(*a*) Compute structure factors F_{hkl}, dielectric susceptibilities χ_{hkl} and absorption coefficients μ/ρ for a given wavelength λ and a range of *hkl* reflexions or for a fixed *hkl* in a given energy range. The atomic scattering factors *f* are interpolated by the program with data from *International Tables for X-ray Crystallography* (1974). The dispersion corrections f' and f'' may be calculated either by a program due to Cromer & Liberman (1970), which is included in *FHKL*, or from data by Henke, Gullikson & Davis (1993) as the user wishes. Thermal agitation (isotropic or anisotropic) may also be taken into account.

(*b*) Draw curves of *f versus* $\sin(\theta)/\lambda$, f' and f'' *versus* energy or μ/ρ *versus* energy.

(*c*) Compute and draw crystal rocking curves in reflexion and transmission cases, taking into account perpendicular or parallel polarization.

(*d*) Perform operations on rocking curves: addition or multiplication by a constant, addition, correlation or convolution of two curves.

Software environment: *FHKL* is designed for Unix workstations. The main program is written in C but some subroutines involving calculations with complex numbers are written in Fortran. An X-window system and OSF-Motif widgets (Xm library) are required for the graphic interface.

Hardware environment: The program has been developed on an IBM RS6000/560 workstation. It also runs on many other Unix computers: it has been compiled successfully on a Hewlett-Packard 9000/735, a Silicon-Graphics Indigo, a Sun-Sparc 4/40 ipc and a PC486 running with Linux. The usual X-window display is necessary.

The memory size of *FHKL* depends on the maximum number of atoms in the crystal cell; for 1000 atoms, a memory of about 6 Mbytes is needed.

Program specification: Note that *FHKL* is usually used for small crystal structures and is not optimized for the calculation of a large number of structure factors in the case of macromolecular structures.

Typical run times for normal utilization are of the order of a few seconds CPU, but in some rare cases it may reach 10 min.

The volume of the source code is estimated as 12 000 lines (including comments) for the C part and 1500 lines for the Fortran subroutines.

Documentation: Documentation of about 900 lines describes the program use and the installation procedure. It is available in the form of an ASCII file or a PostScript file.

Availability: This program is available on request to the author: soyer@lmcp.jussieu.fr. The distribution includes all source codes and documentation and is available by e-mail or ftp. The distribution is free of charge to the research and teaching community.

Keywords: Structure factor, dielectric susceptibility, rocking curve.

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